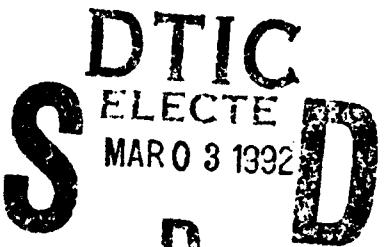


AD-A246 866

(2)

Form Approved
OMB No. 0704-0188

MENTATION PAGE			
1. 1b. RESTRICTIVE MARKINGS			
2a. SECURITY CLASSIFICATION			
2b. DECLASSIFICATION/DOWNGRADING SCHEDULE			
4. PERFORMING ORGANIZATION REPORT NUMBER(S)			
5. MONITORING ORGANIZATION REPORT NUMBER(S)			
6a. NAME OF PERFORMING ORGANIZATION	6b. OFFICE SYMBOL (if applicable)	7a. NAME OF MONITORING ORGANIZATION	
Texas A&M University		Texas A&M Research Foundation	
7b. ADDRESS (City, State, and ZIP Code)			
Department of Chemistry College Station, Texas 77843			
8a. NAME OF FUNDING/SPONSORING ORGANIZATION	8b. OFFICE SYMBOL (if applicable)	9. PROCUREMENT INSTRUMENT IDENTIFICATION NUMBER	
Office of Naval Research	ONR	N00014-89-J-1214	
10. SOURCE OF FUNDING NUMBERS			
PROGRAM ELEMENT NO. PROJECT NO. TASK NO. WORK UNIT ACCESSION NO			
8c. ADDRESS (City, State, and ZIP Code)			
800 North Quincy Street, Code 1513:CF Arlington, VA 22217-5000			
11. TITLE (Include Security Classification) Macrocycles Containing Tin. (Unclassified)			
12. PERSONAL AUTHOR(S) Martin Newcomb			
13a. TYPE OF REPORT Final	13b. TIME COVERED FROM _____ TO _____	14. DATE OF REPORT (Year, Month, Day) 1991, December 31	15. PAGE COUNT 6
16. SUPPLEMENTARY NOTATION			
17. COSATI CODES		18. SUBJECT TERMS (Continue on reverse if necessary and identify by block number) Macrocycle, Anion, Complexation, Structure, Force Field	
FIELD	GROUP	SUB-GROUP	
19. ABSTRACT (Continue on reverse if necessary and identify by block number)			
A summary of project results is reported.			
			
20. DISTRIBUTION/AVAILABILITY OF ABSTRACT		21. ABSTRACT SECURITY CLASSIFICATION	
<input checked="" type="checkbox"/> UNCLASSIFIED/UNLIMITED <input type="checkbox"/> SAME AS RPT <input type="checkbox"/> DTIC USERS		Unclassified	
22a. NAME OF RESPONSIBLE INDIVIDUAL Harold E. Gaurd		22b. TELEPHONE (Include Area Code) (202) 696-1100	22c. OFFICE SYMBOL ONR

OFFICE OF NAVAL RESEARCH

Grant N00014-89-J-1214

R & T Code 4135009

Final Report

by

Martin Newcomb
Department of Chemistry
Wayne State University
Detroit, MI 48202

December 31, 1991

Reproduction in whole or in part is permitted for any purpose of
the United States Government.

This document has been approved for public release
and sale; its distribution is unlimited..

92 2 25 174

92-04938



Macrocycles Containing Tin

The project involved the development of methods for the synthesis, purification and characterization of pre-organized macromolecular hosts containing several Lewis acidic tin atoms, and investigations of the potential for such compounds to bind anions and basic donors selectively. The rationale for the study was that macrocyclic species containing Lewis acidic sites should bind anions and donors within the cavity of the macrocycle in a manner analogous to cation binding by "crown ethers" and "cryptands", and that coordinatively saturated tin atoms, which can become pentacoordinate, are good candidates for the Lewis acids. Selective binding properties that correlate to the fit of an anion or donor in the organized binding region of the macromolecular host were expected, and such properties might be exploited for anion separation, anion identification, and catalysis.

A series of macrobicyclic hosts containing two Lewis acidic tin atoms as binding sites was developed, and anion binding was studied by ^{119}Sn NMR spectroscopy (TR-1, Pub-2). Tricyclic, ditopic hosts containing four Lewis acidic tin atoms were developed (TR-2, Pub-3). X-ray crystal structure determinations of a number of the hosts were obtained (TR-4, TR-5, TR-6, TR-7, TR-8, TR-9, TR-10, TR-11, Pub-5). Solid complexes of macrobicyclic hosts binding anions were isolated and studied by X-ray crystallography and solid state ^{119}Sn NMR spectroscopy (Pub-1). Force field parameters for compounds containing tetrahedral tin atoms were developed and evaluated (TR-3, TR-12, Pub-4). The structures of the macrobicyclic hosts were studied by molecular mechanics calculations, and the results were compared to the crystal structures (TR-13, Pub-5).

Accession For	
NTIS GRA&I	<input checked="" type="checkbox"/>
DTIC TAB	<input type="checkbox"/>
Unannounced	<input type="checkbox"/>
Justification	
By _____	
Distribution:	
Av. Date Rec'd. _____	
Date _____	

A-1

List of Technical Reports

1. "Macrocycles Containing Tin. The Preparation of Macrobicyclic Lewis Acidic Hosts Containing Two Tin Atoms and ^{119}Sn NMR Studies of Their Chloride and Bromide Binding Properties in Solution", Michael T. Blanda, John H. Horner, Martin Newcomb, May 24, 1989
2. "Macrocycles Containing Tin. Ditopic, Tricyclic. Lewis Acidic Hosts with Four Binding Sites", Michael T. Blanda and Martin Newcomb, August 30, 1989
3. "A Preliminary Set of Parameters for Force Field Calculations of Compounds Containing Tetrahedral Tin", John H. Horner and Martin Newcomb*, May 24, 1990
4. "X-Ray Crystal Structure of 1,1,6,6,11,11,16,16-Octaphenyl-1,6,11,16-tetraannaeicosane", Martin Newcomb and John H. Horner, November 7, 1990
5. "X-Ray Crystal Structure of 1,7-Diphenyl-1,7-distannabicyclo[5.5.5]heptadecane", Martin Newcomb and John H. Horner, November 16, 1990
6. "X-Ray Crystal Structure of 1,10-Diphenyl-1,10-distannabicyclo[8.8.8]hexacosane", Martin Newcomb, John H. Horner and Joseph P. Riebenspies, November 21, 1990
7. "X-Ray Crystal Structure of 1,12-Diphenyl-1,12-distannabicyclo[10.10.10]dotriacontane", Martin Newcomb and John H. Horner, November 26, 1990
8. "X-Ray Crystal Structure of 1,7-Dichloro-1,7-distannabicyclo[5.5.5]heptadecane", Martin Newcomb, John H. Horner, Michael T. Blanda, Chau Ha and Phillip J. Squatritto, November 28, 1990
9. "X-Ray Crystal Structure of 1,9-Dichloro-1,9-distannabicyclo[7.7.7]tricosane", Martin Newcomb, John H. Horner, Michael T. Blanda and Nancy McQuire, November 29, 1990
10. "X-Ray Crystal Structure of 1,11-Dichloro-1,11-distannabicyclo[9.9.9]nonacosane" Martin Newcomb and John H. Horner, November 30, 1990
11. "X-Ray Crystal Structure of 1,12-Dichloro-1,12-distannabicyclo[10.10.10]dotriacontane", Martin Newcomb and John H. Horner, December 3, 1990
12. "Parameters for Force Field Calculations of Compounds Containing Tetrahedral Tin", Martin Newcomb and John H. Horner, December 10, 1990
13. "Macrocycles Containing Tin. Crystal Structures and Molecular Mechanics, Calculated Structures of Macrobicyclic Lewis Acidic Hosts", Martin Newcomb and John H. Horner, December 12, 1990

List of Publications:

1. "Macrocycles Containing Tin. Solid Complexes of Anions Encrypted in Macrobicyclic Lewis Acid Hosts", M. Newcomb, J. H. Horner, M. T. Blanda, P. J. Squattrito, *J. Am. Chem. Soc.* **111**, 6294-6301 (1989).
2. "Macrocycles Containing Tin. The Preparation of Macrobicyclic Lewis Acidic Hosts Containing Two Tin Atoms and ^{119}Sn NMR Studies of Their Chloride and Bromide Binding Properties in Solution", M. T. Blanda, J. H. Horner, M. Newcomb, *J. Org. Chem.* **54**, 4626-4636 (1989).
3. "Macrocycles Containing Tin. Lewis Acidic Hosts with Four Binding Sites", M. T. Blanda, M. Newcomb, *Tetrahedron Lett.* **30**, 3501-3504 (1989).
4. "Parameters for Force Field Calculations of Compounds Containing Tetrahedral Tin", J. H. Horner, M. Newcomb, *Organometallics* **10**, 1732-1740 (1991).
5. "Macrocycles Containing Tin. Crystal Structures and Molecular Mechanics Calculated Structures of Macrobicyclic Lewis Acidic Hosts", J. H. Horner, P. J. Squattrito, N. McGuire, J. P. Riebenspies, M. Newcomb, *Organometallics* **10**, 1741-1750 (1991).

List of Personnel

Graduate Students

Dr. Michael T. Blanda
Mr. Paul W. Chambers
Ms. Chau Ha
Ms. Grace Ndip

Post Doctoral Research Associates

Dr. John H. Horner
Dr. M. Udaya Kumar
Dr. Nancy McQuire
Dr. Phillip J. Squatritto

Other Professional Personnel

Dr. J. R. Riebenspies